Chapter 13 - Nuclear Magnetic Resonance Spectroscopy

^{1}H NMR Spectroscopy

We can get similar information from proton NMR that we get from carbon NMR, but there is additional information that we can glean.

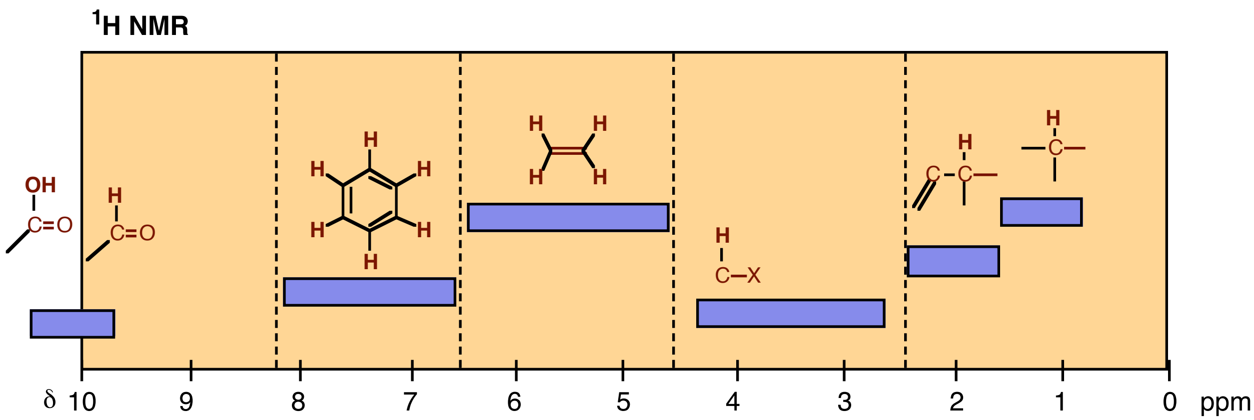
We can see the number of chemically different hydrogens.

We can get the relative ratio of the protons by integration of the area under the peaks.

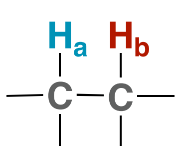
We can tell how many hydrogens are neighboring each resonance through spin-spin splitting (coupling)

Chemical shifts tell us about functional groups.

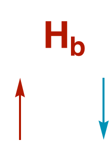
Most proton resonances show up between 0-10 ppm.



Spin-Spin splitting occurs because each proton feels an influence of the neighboring proton spin states. Peaks will be splint into n+1 peaks, where n is the number of H's.

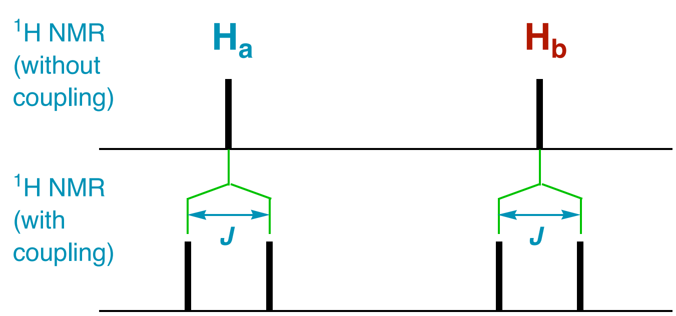


H_a is split into 2 peaks becuase H_b has two spin states, one aligned with the field and one against.

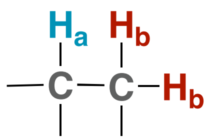


likewise, the H_b proton will be split because of the two spin states of H_a

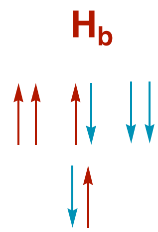
Protons which are coupled to each other will each be split the same distance. This is referred to as the **Coupling Constant (*J*)**



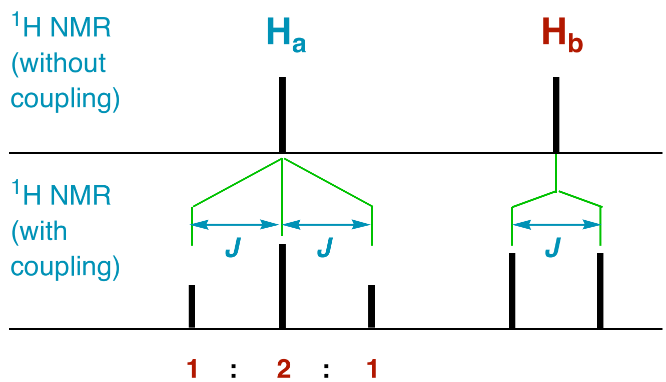
An example of splitting with two neighboring H's.

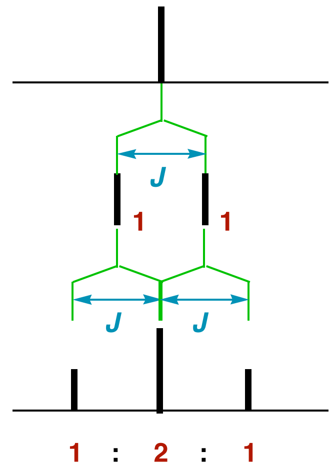


If there are 2 neighboring H's, there are three statistical arrangements of the spin states. In this example, H_a will be split into a triplet.



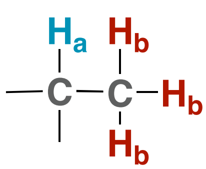
Note that there are two ways to have one spin up and one down. Thus, the middle peak of a triplet will be twice as large as the two outer peaks.



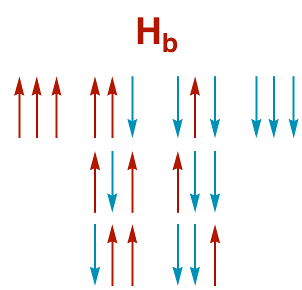


The splitting pattern can be determined by considering one splitting interaction at a time in sequence (reverse tree).

An example of splitting with three neighboring H's.

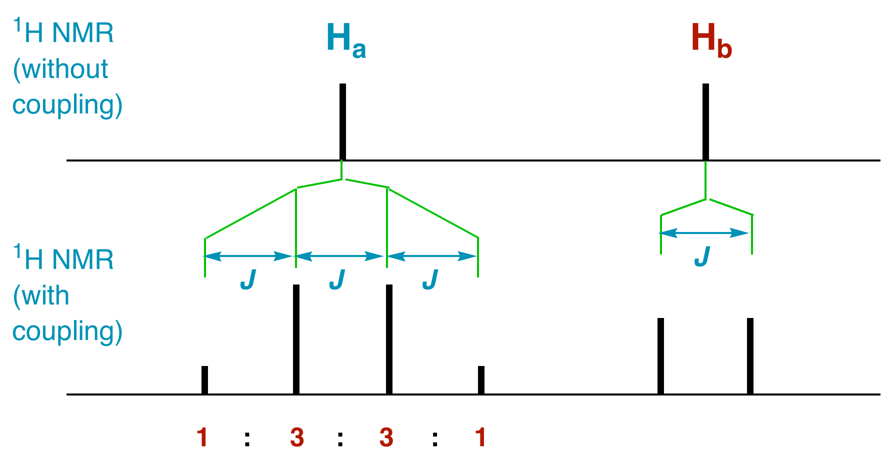


If there are 3 neighboring H's, there are four statistical arrangements of the spin states. In this example, H_a will be split into a quartet.

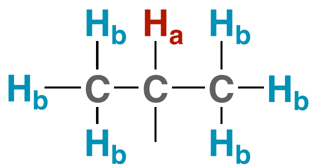


Note the number of statistical arrangements of the various spin states will give rise to a 1:3:3:1 ratio of peaks.

H_a will be a quartet (it sees 3 neighbors) while H_b will remain a doublet (it sees one neighbor)



The relative size of the peaks in a split resonance follows Pascal’s triangle.



H_a will split into 7 peaks

64 different combinations of 6 spins

Pascal's Triangle

singlet	1
doublet	1 1
triplet	1 2 1
quartet	1 3 3 1
quintet	1 4 6 4 1
sextet	1 5 10 10 5 1
septet	1 6 15 20 15 6 1

Summary of simple spin-spin splitting

Proton resonances split into n+1 peaks

Relative ratio of peaks depends on the number of spin states of the neighbor - and follows Pascal’s Triangle.

Adjacent protons couple with the same coupling constant (*J*).

Protons farther away than one carbon do not usually couple

Chemically equivalent protons, even on adjacent carbons, cannot couple. (eg. $Cl\text{-}CH_2CH_2\text{-}Cl$)